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Dynamic range of nanoresonators with random rough surfaces in the presence of thermomechanical and momentum exchange noise

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The authors investigate the simultaneous influence of thermomechanical and momentum exchange noise on the linear dynamic range DR of nanoresonators with random rough surfaces. The latter are characterized by the roughness amplitude w , the lateral correlation length ξ , and the roughness exponent $0 < H < 1$. The dynamic range increases with increasing roughness (decreasing H and/or increasing roughness ratio w/ξ) if the quality factor due to gas collisions is smaller than the intrinsic quality factor associated with thermomechanical noise. The influence of the roughness ratio w/ξ on DR is significant for intermediate roughness exponents that are commonly observed in experiments. © 2007 American Institute of Physics. [DOI: 10.1063/1.2751599]

With the advent of nanoelectromechanical systems (NEMSs), an important class of devices was introduced, which combines the advantages of mechanical systems, e.g., applicability as sensor systems and robustness to electrical shocks, with the speed and large scale integration of silicon electronics.^{1–3} Moreover, NEMSs are mostly operated in the linear response regime, where the dynamics remains well controlled. However, if the driving amplitude of a resonator is enhanced, the system might be driven into the nonlinear or chaotic regime.⁴ For NEMS in sensing or switching signals, it is quite important to determine the possibility and the specific kind of linear to nonlinear transition.⁵

The linear dynamic range (DR) is an established concept to characterize the linear behavior of nanoresonators. It originates from amplifier studies, expressing the window of input power where the amplifier behaves linearly.^{6,7} The bottom of DR is determined by the noise power generated within the amplifier and the top by the input power level at which 1 dB compression occurs. Correspondingly, the DR for a nanoresonator is defined as the ratio of its maximum vibration amplitude $\langle x_c \rangle$ at the onset of nonlinearity to its rms displacement noise floor $\int S(\omega) d\omega$ within the operation bandwidth Δf so that^{6,7}

$$\text{DR} = 10 \log \left[\frac{\langle x_c \rangle^2}{\int_{\omega_o - \pi \Delta f}^{\omega_o + \pi \Delta f} S(\omega) d\omega} \right]. \quad (1)$$

A complete treatment of DR must include thermomechanical noise, momentum exchange, readout noise, and in more general any contributing noise sources in the displacement spectral noise density $S(\omega)$. Thermomechanical noise arises from coupling between a mechanical resonator and its dissipative reservoir. The coupling damps the resonator motion and induces spatial fluctuations in the resonator's position at non-zero temperature (peaking at the mechanical resonance frequencies).^{8,9} It could be a dominant source of frequency noise at a given mode of vibration, and it imposes an ultimate limit of detection for a dynamic micromechanical sensor.^{8,10,11} Notably, due to its small heat capacity, a nan-

oresonator can be subject to rather large temperature fluctuations (which induce frequency fluctuations because dimensions and material parameters are both temperature dependent).⁶ The latter depend on the thermal coupling strength to the environment.⁶ Furthermore, the resonator can undergo gas damping due to impingement and momentum exchange of surrounding gas molecules on the resonator surface.^{6,12,13} In addition, mass loading takes due to adsorption-desorption of gas molecules (parametric noise leaving unaffected the quality factor).^{3,6,11,14}

Studies of SiC/Si NEMS have shown that devices operational in the UHF/microwave regime have low surface roughness, while devices with rougher surfaces cannot be operated higher than the VHF regime.¹⁵ Other studies of Si nanowires have shown the quality factor to decrease by an increment of the surface area to volume ratio.¹⁶ Recently, random surface roughness was shown to affect the quality factor and the limit to mass sensitivity of nanoresonators.^{12,14} The previous studies showed that surface effects play a dominant role in NEMS and likely affect their dynamic range. Therefore, in the present work we will consider the influence of surface roughness on the resonator dynamic range DR in the presence of thermomechanical noise generated by the internal loss mechanisms in the resonator and momentum exchange noise generated from impinging surrounding gas molecules. Both types of noise lead to direct random displacements of the resonator. Modeling of the surface roughness will be considered for the case of self-affine random roughness, which is observed in a wide variety of surface engineering procedures.¹⁷

For thermomechanical noise, the spectral density of random displacements is given by⁵ $S(\omega)_{\text{thm}} = (4\omega_o K_B T / M_{\text{eff}} Q_{\text{in}}) \times [(\omega^2 - \omega_o^2)^2 + (\omega\omega_o)^2 / Q_{\text{in}}^2]^{-1}$, with Q_{in} the intrinsic quality factor of the resonator. For momentum exchange noise, the noise spectral density is given by $S(\omega)_{\text{mexh}} = (4\omega_o K_B T / M_{\text{eff}} Q_{\text{gas}}) [(\omega^2 - \omega_o^2)^2 + (\omega\omega_o)^2 / Q_{\text{gas}}^2]^{-1}$ (Refs. 3, 6, and 11) assuming that the resonator operates in the molecular regime. The latter means a molecule mean free path L_{mph} larger than the resonator width w_b (assuming also $w_b \ll L$ with L beam length).¹³ Q_{gas} is the quality factor due to gas damping. Furthermore, the noise spectrum by the combined effect of both noise terms has the form $S(\omega)$,

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$= (4\omega_o K_B T / M_{\text{eff}} Q_t) [(\omega^2 - \omega_o^2)^2 + (\omega\omega_o)^2 / Q_t^2]^{-1}$, where $1/Q_t = 1/Q_{\text{in}} + 1/Q_{\text{gas}}$ and Q_t representing the total quality factor of the system.

Substitution of the spectral density $S(\omega)_t$ in Eq. (1) yields for the dynamic range $\text{DR} = 10 \{ \log[(E_c / K_B T) \times (\omega_o / 4Q_{\text{in}} \Delta f)] + \log[1 + (Q_{\text{in}} / Q_{\text{gas}})] \}$ assuming that $Q_t \gg 1$ and $\omega_o / Q_{\text{it}} \gg 2\pi \Delta f$.⁶ $Q_{\text{gas}} = M_{\text{eff}} \omega_o \sqrt{K_B T / m} (\text{PA}_{\text{rou}})^{-1}$, with $v_T = (K_B T / m)^{1/2}$ the thermal molecule velocity, m the molecule mass, M_{eff} the effective resonator mass that oscillates, and A_{rou} the rough surface area of the resonator.¹² If we assume for the roughness profile a single valued random function $h(r)$ of the in-plane position $r = (x, y)$ and a Gaussian height distribution, the rough area is given by $A_{\text{rou}} / A_{\text{flat}} = \int_0^{+\infty} du (\sqrt{1 + \rho^2 u}) e^{-u}$,¹⁸ with $\rho = \sqrt{\langle (\nabla h)^2 \rangle}$ the average local surface slope $[\rho = (\int_0^{+\infty} q^2 \langle |h(q)|^2 \rangle > d^2 q)^{1/2}]$,¹⁹ and $A_{\text{flat}} = 2w_b L$ is the average flat surface area. $Q_c = \pi / a_o$ with a_o a lower lateral cutoff. Finally, $\langle |h(q)|^2 \rangle$ is the roughness spectrum. Upon substitution we obtain for the dynamic range DR

$$\text{DR} = \text{DR}_{\text{flat}} + 10 \times \log \left[1 + (Q_{\text{in}} / Q_{\text{gas},f}) \int_0^{+\infty} du (\sqrt{1 + \rho^2 u}) e^{-u} \right], \quad (2)$$

with $\text{DR}_{\text{flat}} = 10 \{ \log[(E_c / K_B T) (\omega_o / 4Q_{\text{in}} \Delta f)] \}$ and $Q_{\text{gas},f} = M_{\text{eff}} \omega_o \sqrt{K_B T / m} / (\text{PA}_{\text{flat}})$.

Calculations of DR by means of Eq. (2) requires knowledge of the roughness spectrum $\langle |h(q)|^2 \rangle$. Indeed, a wide variety of surfaces possesses the so-called self-affine roughness^{15,18} with a roughness spectrum that scales as $\langle |h(q)|^2 \rangle \propto q^{-2-2H}$ if $q\xi \gg 1$ and $\langle |h(q)|^2 \rangle \propto \text{const}$ if $q\xi \ll 1$.^{17,20} This is satisfied by the analytic model²⁰ $\langle |h(q)|^2 \rangle = (2\pi w^2 \xi^2) / (1 + a q^2 \xi^2)^{(1+H)}$ with $a = (1/2H)[1 - (1 + a Q_c^2 \xi^2)^{-H}]$ if $0 < H < 1$ and $a = 1/2 \ln(1 + a Q_c^2 \xi^2)$ if $H = 0$. Small values of H (~ 0) characterize jagged or irregular surfaces, while large values of H (~ 1) surfaces with smooth hills and valleys.^{17,20} For other roughness models, see Ref. 21. In addition, we obtain for the local slope $\rho = (w / \sqrt{2\xi a}) \sqrt{(1-H)^{-1} [(1 + a Q_c^2 \xi^2)^{1-H} - 1] - 2a}$.¹⁹

Our calculations were performed for roughness amplitudes observed in real resonators in the range $w \sim 2-8$ nm,¹⁵ and $a_o = 0.3$ nm. Figure 1 shows calculations of the linear dynamic range DR as a function of the long wavelength roughness ratio w/ξ . It is evident that the dynamic range DR increases as the surface becomes rougher (lower roughness exponents H and/or larger ratio w/ξ). In this case, the quality factor imposed by the gas collisions will decrease and start playing a significant role in the resonator motion or even in getting the dominant dissipation term. Notably with decreasing roughness exponent H , the increment of DR with increasing ratio w/ξ becomes drastically fast.

The direct dependence on the roughness exponent H is shown in Fig. 2, where the fast saturation of DR at the flat surface value $(\text{DR} - \text{DR}_{\text{flat}}) \equiv \log[1 + Q_{\text{in}} / Q_{\text{gas},f}]$ for large roughness exponents ($H \sim 1$) becomes clear. On the other hand, at small roughness exponents ($H \sim 0$) the influence of the ratio w/ξ is strongly diminished. In fact, the influence of the ratio w/ξ becomes more distinct in the intermediate range of roughness exponents $0.3 < H < 0.8$, which are the more commonly observed exponents in experimental systems.¹⁷

FIG. 1. DR as a function of the long wavelength roughness ratio w/ξ , for $w = 3$ nm, and various exponents H , as indicated. (a) $Q_{\text{in}}/Q_{\text{gas},f} = 1$ and (b) $Q_{\text{in}}/Q_{\text{gas},f} = 0.1$.

Furthermore, as Fig. 3(a) indicates with decreasing quality ratio $Q_{\text{in}}/Q_{\text{gas},f}$ (or increasing gas dissipation), the dynamic range DR becomes more sensitive to roughness changes as the topmost curve indicates for $Q_{\text{in}} < Q_{\text{gas},f}$. The latter is also directly shown in Fig. 3(b) for various roughness exponents H . In comparison with the effect of the adsorption-desorption noise, where increasing roughness de-

FIG. 2. (Color online) DR as a function of the ratio w/ξ , for $w = 3$ nm, $Q_{\text{in}}/Q_{\text{gas},f} = 1$, and H , as indicated.

FIG. 3. (a) DR vs w/ξ , for $w=3$ nm, $H=0.5$, and ratios $Q_{in}/Q_{gas,f}$ as indicated. (b) DR vs $Q_{in}/Q_{gas,f}$ for $\xi=100$ nm, for $w=3$ nm, and H , as indicated.

creases DR (because the noise floor is proportional to the rough surface area),¹⁴ the momentum exchange noise has the inverse effect and increases DR when $Q_{gas,f} < Q_{in}$. In the opposite limit for $Q_{in}Q_{gas,f}$ [where the roughness influence is weak, e.g., Fig. 3(a)] by considering the asymptotic expansion $\log(1+y) = \sum_{m=0,\infty} [(-1)^m / (1+m)] y^{1+m} / \ln(10)$ and weak local slopes ($\rho \ll 1$) so that $\int_0^{+\infty} du (\sqrt{1+\rho^2 u}) e^{-u} \approx 1 + (\rho^2/2)$, we obtain the analytic form (as series expansion) $DR = DR_{flat} + [10/\ln(10)] \sum_{m=0,\infty} [(-1)^m / (1+m)] \times (Q_{in}/Q_{gas,f})^{1+m} [1 + (1+m)\rho^2/2]$.

In conclusion, we investigated the simultaneous influence of thermomechanical and momentum exchange noise on the linear dynamic range of nanoresonators. With increasing surface roughness, the linear dynamic range increases significantly if the quality factor due to gas collisions is comparable or smaller than the intrinsic quality factor associated

with thermomechanical noise. In addition, the influence of the roughness ratio w/ξ on the dynamic range becomes more distinct in the intermediate range of exponents $0.3 < H < 0.8$ that are commonly observed in experiments. In any case, our results translate into a clear indication that the surface morphology could play a significant role on the dynamic range of nanoresonators, and further studies are necessary to account for more complex noise contributions.

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